

Mathematical and Statistical Methods in Food Science and Technology

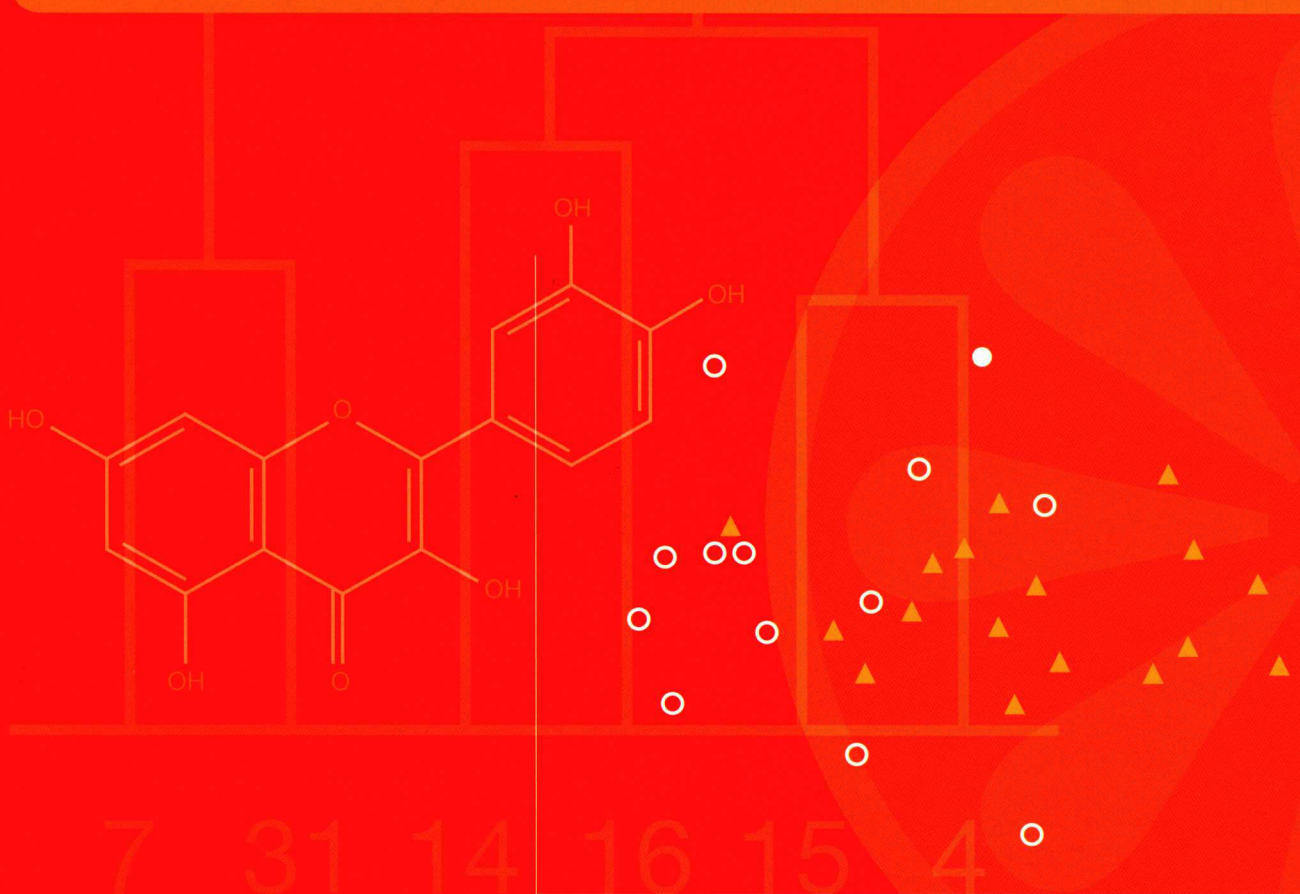
Daniel Granato and
Gastón Ares

EDITORS



Press

WILEY Blackwell



Mathematical and Statistical Methods in Food Science and Technology

Edited by

Daniel Granato

*Food Science and Technology Graduate Programme, State University of Ponta Grossa,
Ponta Grossa, Brazil*

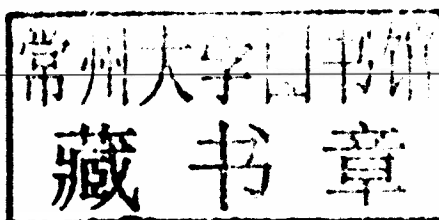
Gastón Ares

Department of Food Science and Technology, Universidad de la República, Montevideo, Uruguay



| Press

WILEY Blackwell



This edition first published 2014 ©2014 by John Wiley & Sons, Ltd

Registered office: John Wiley & Sons, Ltd, The Atrium, Southern Gate, Chichester, West Sussex, PO19 8SQ, UK

Editorial offices: 9600 Garsington Road, Oxford, OX4 2DQ, UK
The Atrium, Southern Gate, Chichester, West Sussex, PO19 8SQ, UK
111 River Street, Hoboken, NJ 07030-5774, USA

For details of our global editorial offices, for customer services and for information about how to apply for permission to reuse the copyright material in this book please see our website at www.wiley.com/wiley-blackwell.

The right of the author to be identified as the author of this work has been asserted in accordance with the UK Copyright, Designs and Patents Act 1988.

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, recording or otherwise, except as permitted by the UK Copyright, Designs and Patents Act 1988, without the prior permission of the publisher.

Designations used by companies to distinguish their products are often claimed as trademarks. All brand names and product names used in this book are trade names, service marks, trademarks or registered trademarks of their respective owners. The publisher is not associated with any product or vendor mentioned in this book.

Limit of Liability/Disclaimer of Warranty: While the publisher and author(s) have used their best efforts in preparing this book, they make no representations or warranties with respect to the accuracy or completeness of the contents of this book and specifically disclaim any implied warranties of merchantability or fitness for a particular purpose. It is sold on the understanding that the publisher is not engaged in rendering professional services and neither the publisher nor the author shall be liable for damages arising herefrom. If professional advice or other expert assistance is required, the services of a competent professional should be sought.

Library of Congress Cataloging-in-Publication Data

Mathematical and statistical methods in food science and technology / edited
by Daniel Granato and Gaston Ares.

pages cm

Includes bibliographical references and index.

ISBN 978-1-118-43368-3 (cloth)

1. Food—Analysis—Statistical methods. 2. Food
contamination—Research—Statistical methods. 3. Food supply—Mathematics.
I. Granato, Daniel, editor of compilation. II. Ares, Gaston, editor of
compilation.

TX541.M377 2013

664'.07—dc23

2013026555

A catalogue record for this book is available from the British Library.

Wiley also publishes its books in a variety of electronic formats. Some content that appears in print may not be available in electronic books.

Cover design and illustration by www.hisandhersdesign.co.uk

Set in 10/12pt, Times by Thomson Digital, Noida, India.
Printed and bound in Malaysia by Vivar Printing Sdn Bhd

Mathematical and Statistical Methods in Food Science and Technology



The *IFT Press* series reflects the mission of the Institute of Food Technologists — to advance the science of food contributing to healthier people everywhere. Developed in partnership with Wiley Blackwell, *IFT Press* books serve as leading-edge handbooks for industrial application and reference and as essential texts for academic programs. Crafted through rigorous peer review and meticulous research, *IFT Press* publications represent the latest, most significant resources available to food scientists and related agriculture professionals worldwide. Founded in 1939, the Institute of Food Technologists is a nonprofit scientific society with 18,000 individual members working in food science, food technology, and related professions in industry, academia, and government. IFT serves as a conduit for multidisciplinary science thought leadership, championing the use of sound science across the food value chain through knowledge sharing, education, and advocacy.

IFT Press Advisory Group

Nicolas Bordenave
YiFang Chu
J. Peter Clark
Christopher J. Doona
Jung Hoon Han
Florence Feeherry
Chris Findlay
David McDade
Thomas J. Montville
Karen Nachay
Martin Okos
David S. Reid
Sam Saguy
Fereidoon Shahidi
Cindy Stewart
Herbert Stone
Kenneth R. Swartzel
Bob Swientek
Hilary Thesmar
Yael Vodovotz
Ron Wrolstad

WILEY Blackwell

Titles in the IFT Press series

- *Accelerating New Food Product Design and Development* (Jacqueline H. Beckley, Elizabeth J. Topp, M. Michele Foley, J.C. Huang, and Witoon Prinyawiwatkul)
- *Advances in Dairy Ingredients* (Geoffrey W. Smithers and Mary Ann Augustin)
- *Bioactive Proteins and Peptides as Functional Foods and Nutraceuticals* (Yoshinori Mine, Eunice Li-Chan, and Bo Jiang)
- *Biofilms in the Food Environment* (Hans P. Blaschek, Hua H. Wang, and Meredith E. Agle)
- *Calorimetry in Food Processing: Analysis and Design of Food Systems* (Gönül Kaletunç)
- *Coffee: Emerging Health Effects and Disease Prevention* (YiFang Chu)
- *Food Carbohydrate Chemistry* (Ronald E. Wrolstad)
- *Food Ingredients for the Global Market* (Yao-Wen Huang and Claire L. Kruger)
- *Food Irradiation Research and Technology*, Second Edition (Christopher H. Sommers and Xuetong Fan)
- *Foodborne Pathogens in the Food Processing Environment: Sources, Detection and Control* (Sadhana Ravishankar, Vijay K. Juneja, and Divya Jaroni)
- *High Pressure Processing of Foods* (Christopher J. Doona and Florence E. Feeherry)
- *Hydrocolloids in Food Processing* (Thomas R. Laaman)
- *Improving Import Food Safety* (Wayne C. Ellefson, Lorna Zach, and Darryl Sullivan)
- *Innovative Food Processing Technologies: Advances in Multiphysics Simulation* (Kai Knoerzer, Pablo Juliano, Peter Roupas, and Cornelis Versteeg)
- *Microbial Safety of Fresh Produce* (Xuetong Fan, Brendan A. Niemira, Christopher J. Doona, Florence E. Feeherry, and Robert B. Gravani)
- *Microbiology and Technology of Fermented Foods* (Robert W. Hutkins)
- *Multiphysics Simulation of Emerging Food Processing Technologies* (Kai Knoerzer, Pablo Juliano, Peter Roupas and Cornelis Versteeg)
- *Multivariate and Probabilistic Analyses of Sensory Science Problems* (Jean-François Meullenet, Rui Xiong, and Christopher J. Findlay)
- *Nanoscience and Nanotechnology in Food Systems* (Hongda Chen)
- *Natural Food Flavors and Colorants* (Mathew Attokaran)
- *Nondestructive Testing of Food Quality* (Joseph Irudayaraj and Christoph Reh)
- *Nondigestible Carbohydrates and Digestive Health* (Teresa M. Paeschke and William R. Aimutis)
- *Nonthermal Processing Technologies for Food* (Howard Q. Zhang, Gustavo V. Barbosa-Cánovas, V.M. Balasubramaniam, C. Patrick Dunne, Daniel F. Farkas, and James T.C. Yuan)
- *Nutraceuticals, Glycemic Health and Type 2 Diabetes* (Vijai K. Pasupuleti and James W. Anderson)
- *Organic Meat Production and Processing* (Steven C. Ricke, Ellen J. Van Loo, Michael G. Johnson, and Corliss A. O' Bryan)
- *Packaging for Nonthermal Processing of Food* (Jung H. Han)
- *Practical Ethics for Food Professionals: Ethics in Research, Education and the Workplace* (J. Peter Clark and Christopher Ritson)
- *Preharvest and Postharvest Food Safety: Contemporary Issues and Future Directions* (Ross C. Beier, Suresh D. Pillai, and Timothy D. Phillips, Editors; Richard L. Ziprin, Associate Editor)
- *Processing and Nutrition of Fats and Oils* (Ernesto M. Hernandez and Afaf Kamal-Eldin)
- *Processing Organic Foods for the Global Market* (Gwendolyn V. Wyard, Anne Plotto, Jessica Walden, and Kathryn Schuett)
- *Regulation of Functional Foods and Nutraceuticals: A Global Perspective* (Clare M. Hasler)
- *Resistant Starch: Sources, Applications and Health Benefits* (Yong-Cheng Shi and Clodualdo Maningat)

- *Sensory and Consumer Research in Food Product Design and Development* (Howard R. Moskowitz, Jacqueline H. Beckley, and Anna V.A. Resurreccion)
- *Sustainability in the Food Industry* (Cheryl J. Baldwin)
- *Thermal Processing of Foods: Control and Automation* (K.P. Sandeep)
- *Trait - Modified Oils in Foods* (Frank T. Orthoefer and Gary R. List)
- *Water Activity in Foods: Fundamentals and Applications* (Gustavo V. Barbosa-Cánovas, Anthony J. Fontana Jr., Shelly J. Schmidt, and Theodore P. Labuza)
- *Whey Processing, Functionality and Health Benefits* (Charles I. Onwulata and Peter J. Huth)

WILEY Blackwell

About the editors



Daniel Granato is a Food Engineer. He completed his Master's degree in Food Technology (Federal University of Paraná, Brazil) in 2009 and undertook his Doctoral degree in Food Science (University of São Paulo, Brazil) from 2009–2011. In his Master's dissertation, he used Response Surface Methodology (RSM) to model and optimize physico-chemical and sensory properties of a dairy-free dessert. In his PhD thesis, he used multivariate statistical techniques to assess the influence of the grape variety, origin, price, sensory properties, *in vitro* antioxidant capacity, instrumental colour and chemical composition of red wines from South America on *in vivo* antioxidant activity (using Wistar rats). He has worked at the Adolfo Lutz Institute (São Paulo, Brazil) as a Researcher in the Department of Analysis and Data Processing since 2012. He has authored more than 40 articles in international refereed journals and various presentations at Con-

gresses. He has worked and collaborated with many research groups in the following fields: food safety, food development/optimization using RSM, chemistry, sensory analysis, chemometrics and sensometrics applied in food science and technology. He is an active reviewer of more than 30 scientific peer-reviewed journals.



Gastón Ares is a Food Engineer. He received his PhD in chemistry, focusing on sensory and consumer science, from the Universidad de la República (Uruguay) in 2009. He has worked as professor and researcher in the Food Science and Technology Department of the Chemistry Faculty of the Universidad de la República (Uruguay) since 2005. His research has been focused on the application of novel methodologies for the development and evaluation of food products and processes. He has extensive experience in the application of multivariate statistical and mathematical techniques. He has authored more than 80 articles in international refereed journals and numerous presentations in scientific meetings. He was awarded the 2007 Rose Marie Pangborn Sensory Science Scholarship, granted to PhD students in sensory science worldwide. In 2011 he won the Food Quality and Preference Award for a young researcher for his contributions to

sensory and consumer science, and the Scopus Uruguay Award in Engineering and Technology. He is member of the Editorial Boards of both the *Journal of Sensory Studies* and the journal *Food Quality and Preference*, as well as associate editor of *Food Research International*.

List of contributors

Azila Abdul-Aziz, Institute of Bioproduct Development, Universiti Teknologi Malaysia, Skudai Johor, Malaysia

José Manuel Amigo, Department of Food Science, Faculty of Sciences, University of Copenhagen, Frederiksberg, Denmark

Gastón Ares, Department of Food Science and Technology, Facultad de Química, Universidad de la República, Montevideo, Uruguay

Ramlan Aziz, Institute of Bioproduct Development, Universiti Teknologi Malaysia, Skudai Johor, Malaysia

Andreas Baierl, Department of Statistics and Operations Research, University of Vienna, Vienna, Austria

Débora Cristiane Bassani, Department of Biomedicine, Centro Educacional das Faculdades Metropolitanas Unidas, São Paulo, SP, Brazil

Francis Butler, School of Biosystems Engineering, Agriculture and Food Science Centre, University College Dublin, Belfield, Dublin 4, Ireland

Vasco Augusto Pilão Cadavez, CIMO Mountain Research Centre, School of Agriculture (ESA) of the Polytechnic Institute of Bragança (IPB), Bragança, Portugal

Shin-Kyo Chung, School of Food Science & Biotechnology, Kyungpook National University, Daegu, Republic of Korea

Maria G. Corradini, Department of Food Science, Rutgers, The State University of New Jersey, New Brunswick, NJ, USA

Daniel Cozzolino, School of Agriculture, Food and Wine, Faculty of Sciences, The University of Adelaide, Waite Campus, Glen Osmond, SA, Australia

Verônica Maria de Araújo Calado, Escola de Química, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil

Eva Derndorfer, University of Applied Sciences Burgenland, University of Salzburg, UMIT Hall in Tirol, and independent sensory consultant, Vienna, Austria

Rolf Ergon, Telemark University College, Porsgrunn, Norway

Tamas Ferenci, Physiological Control Group, Institute of Information Systems, John von Neumann Faculty of Informatics, Obuda University, Budapest, Hungary

Ursula Andrea Gonzales-Barron, CIMO Mountain Research Centre, School of Agriculture (ESA) of the Polytechnic Institute of Bragança (IPB), Bragança, Portugal

Daniel Granato, Food Science and Technology Graduate Programme, State University of Ponta Grossa, Ponta Grossa, Brazil

Aurea Grané, Statistics Department, Universidad Carlos III de Madrid, Getafe, Spain

Jos A. Hageman, Plant Sciences Group, Wageningen UR, Wageningen, The Netherlands

Noor Hafiza Harun, Institute of Bioproduct Development, Universiti Teknologi Malaysia, Skudai Johor, Malaysia

Anthony D. Hitchins, Rockville, MD, USA [Center for Food Safety and Applied Nutrition, United States Food and Drug Administration (retired)]

François Husson, Laboratoire de mathématiques appliquées, Agrocampus Ouest, Rennes Cedex, France

Agnieszka Jach, Statistics Department, Universidad Carlos III de Madrid, Getafe, Spain

Jeffrey E. Jarrett, University of Rhode Island, Kingston, RI, USA

Basil Jarvis, Department of Food and Nutrition Sciences, School of Chemistry, Food and Pharmacy, The University of Reading, Whiteknights, Reading, Berkshire, UK

Jasenka Gajdos Kljusuric, Faculty of Food Technology and Biotechnology, University of Zagreb, Zagreb, Croatia

Levente Kovacs, Physiological Control Group, Institute of Information Systems, John von Neumann Faculty of Informatics, Obuda University, Budapest, Hungary

Zelimir Kurtanjek, Faculty of Food Technology and Biotechnology, University of Zagreb, Zagreb, Croatia

João A. Lopes, REQUIMTE, Laboratório de Análises Químicas e Físico-Químicas, Departamento de Ciências Químicas, Faculdade de Farmácia, Universidade do Porto, Porto, Portugal

Mohd Faizal Muhammad, Institute of Bioproduct Development, Universiti Teknologi Malaysia, Skudai Johor, Malaysia

Sulaiman Ngadiran, Institute of Bioproduct Development, Universiti Teknologi Malaysia, Skudai Johor, Malaysia

Mark D. Normand, Department of Food Science, Chenoweth Laboratories, University of Massachusetts, Amherst, MA, USA

Domingos Sávio Nunes, Department of Chemistry, Universidade Estadual de Ponta Grossa, Ponta Grossa, PR, Brazil

Massimo Pacella, Dipartimento di Ingegneria dell'Innovazione, Università del Salento, Lecce, Italy

Jérôme Pagès, Laboratoire de mathématiques appliquées, Agrocampus Ouest, Rennes Cedex, France

Micha Peleg, Department of Food Science, Chenoweth Laboratories, University of Massachusetts, Amherst, MA, USA

Fernando Pérez-Rodríguez, Department of Food Science and Technology, University of Cordoba – International Campus of Excellence in the AgriFood Sector ceiA3, Campus Rabanales, Edificio Darwin – Córdoba, Spain

Roshanida Abdul Rahman, Faculty of Chemical Engineering, Universiti Teknologi Malaysia, Skudai Johor, Malaysia

Marco S. Reis, CIEPQPF, Department of Chemical Engineering, University of Coimbra, Coimbra, Portugal

Åsmund Rinnan, Department of Food Science, Faculty of Science, University of Copenhagen, Frederiksberg, Denmark

Ernie Surianiy Rosly, Institute of Bioproduct Development, Universiti Teknologi Malaysia, Skudai Johor, Malaysia

Quirico Semeraro, Dipartimento di Meccanica, Politecnico di Milano, Milan, Italy

Thomas Skov, Department of Food Science, Faculty of Science, University of Copenhagen, Frederiksberg, Denmark

Clara C. Sousa, REQUIMTE, Laboratório de Microbiologia, Departamento de Ciências Biológicas, Faculdade de Farmácia, Universidade do Porto, Porto, Portugal

Panagiotis H. Tsarouhas, Department of Standardization & Transportation of Products – Logistics, Alexander Technological Educational Institute of Thessaloniki, Katerini, Greece

Grishja van der Veer, RIKILT Institute of Food Safety, Wageningen UR, Wageningen, The Netherlands

Saskia M. van Ruth, Product Design and Quality Group, Wageningen UR and RIKILT Institute of Food Safety, Wageningen UR, Wageningen, The Netherlands

Paula Varela, Propiedades físicas y sensoriales de alimentos y ciencia del consumidor, Instituto de Agroquímica y Tecnología de Alimentos (CSIC), Paterna (Valencia), Spain

Wan Mastura Wan Zamri, Institute of Bioproduct Development, Universiti Teknologi Malaysia, Skudai Johor, Malaysia

Harisun Yaakob, Institute of Bioproduct Development, Universiti Teknologi Malaysia, Skudai Johor, Malaysia

Hu-Zhe Zheng, Department of Food & Nutrition Engineering, Jiangsu Food & Pharmaceutical Science College, Jiangsu Huai'an, China

Acknowledgements

Firstly, I need to thank God that I am here doing what I love: research. All people I love are part of this book and I dedicate this effort to them: Maria Aparecida Granato, Marcos Granato, Gustavo Granato, Felipe Borges, and all my dearest friends. Thank you for understanding and supporting me, no matter what.

I also would like to thank Professor Dr Anderson Sant'Ana for suggesting some of the topics covered in this book and for his support. I want to thank all authors who accepted the invitation to contribute to this book.

Daniel Granato

Thanks to all the authors for joining the project and providing high-quality contributions.

On a personal level I would like to thank my family and friends for their continuous love and support. Thanks for giving me the strength to achieve all my dreams.

Gastón Ares

Contents

<i>About the editors</i>	xi
<i>List of contributors</i>	xiii
<i>Acknowledgements</i>	xvii
Section 1	1
1 The use and importance of design of experiments (DOE) in process modelling in food science and technology	3
<i>Daniel Granato and Verônica Maria de Araújo Calado</i>	
2 The use of correlation, association and regression to analyse processes and products	19
<i>Daniel Cozzolino</i>	
3 Case study: Optimization of enzyme-aided extraction of polyphenols from unripe apples by response surface methodology	31
<i>Hu-Zhe Zheng and Shin-Kyo Chung</i>	
4 Case study: Statistical analysis of eurycomanone yield using a full factorial design	43
<i>Azila Abdul-Aziz, Harisun Yaakob, Ramlan Aziz, Roshanida Abdul Rahman, Sulaiman Ngadiran, Mohd Faizal Muhammad, Noor Hafiza Harun, Wan Mastura Wan Zamri and Ernie Surianiy Rosly</i>	
Section 2	55
5 Applications of principal component analysis (PCA) in food science and technology	57
<i>Aurea Grané and Agnieszka Jach</i>	
6 Multiple factor analysis: Presentation of the method using sensory data	87
<i>Jérôme Pagès and François Husson</i>	
7 Cluster analysis: Application in food science and technology	103
<i>Gastón Ares</i>	
8 Principal component regression (PCR) and partial least squares regression (PLSR)	121
<i>Rolf Ergon</i>	
9 Multiway methods in food science	143
<i>Åsmund Rinnan, José Manuel Amigo and Thomas Skov</i>	

10	Multidimensional scaling (MDS)	175
	<i>Eva Derndorfer and Andreas Baierl</i>	
11	Application of multivariate statistical methods during new product development – Case study: Application of principal component analysis and hierarchical cluster analysis on consumer liking data of orange juices	187
	<i>Paula Varela</i>	
12	Multivariate image analysis	201
	<i>Marco S. Reis</i>	
13	Case Study: Quality control of <i>Camellia sinensis</i> and <i>Ilex paraguariensis</i> teas marketed in Brazil based on total phenolics, flavonoids and free-radical scavenging activity using chemometrics	219
	<i>Débora Cristiane Bassani, Domingos Sávio Nunes and Daniel Granato</i>	
Section 3		231
14	Statistical approaches to develop and validate microbiological analytical methods	233
	<i>Anthony D. Hitchins</i>	
15	Statistical approaches to the analysis of microbiological data	249
	<i>Basil Jarvis</i>	
16	Statistical modelling of anthropometric characteristics evaluated on nutritional status	285
	<i>Zelimir Kurtanek and Jasenka Gajdos Kljusuric</i>	
17	Effects of paediatric obesity: a multivariate analysis of laboratory parameters	303
	<i>Tamas Ferenci and Levente Kovacs</i>	
18	Development and application of predictive microbiology models in foods	321
	<i>Fernando Pérez-Rodríguez</i>	
19	Statistical approaches for the design of sampling plans for microbiological monitoring of foods	363
	<i>Ursula Andrea Gonzales-Barron, Vasco Augusto Pilão Cadavez and Francis Butler</i>	
20	Infrared spectroscopy detection coupled to chemometrics to characterize foodborne pathogens at a subspecies level	385
	<i>Clara C. Sousa and João A. Lopes</i>	
Section 4		419
21	Multivariate statistical quality control	421
	<i>Jeffrey E. Jarrett</i>	

22	Application of neural-based algorithms as statistical tools for quality control of manufacturing processes	431
	<i>Massimo Pacella and Quirico Semeraro</i>	
23	An integral approach to validation of analytical fingerprinting methods in combination with chemometric modelling for food quality assurance	449
	<i>Grishja van der Veer, Saskia M. van Ruth and Jos A. Hageman</i>	
24	Translating randomly fluctuating QC records into the probabilities of future mishaps	471
	<i>Micha Peleg, Mark D. Normand and Maria G. Corradini</i>	
25	Application of statistical approaches for analysing the reliability and maintainability of food production lines: a case study of mozzarella cheese	491
	<i>Panagiotis H. Tsarouhas</i>	
	<i>Index</i>	511

Section 1
